# A Computational Evaluation the Factors Affecting the Structure of α– and β–D-Glucopyanose in Vacuum

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The cyclic structures of α– and β–D-glucopyranose differ in energy by less than a kcal (~0.3 kcal at 298 K in aqueous solution) and both the α– and β– conformers have several relatively stable rotamers in solution. These rotamers are referred to as *gg*, *gt*, and *tg* according to the position of the –OH attached to the -$CH_2$ at position C5 on the ring. While the axial versus equatorial orientation of the hydroxyl group at C1 gives rise to the conformational energy, the energies of the *gg*, *gt*, and *tg* rotamers are based on the orientation of the hydroxymethyl group at C5.

Relaxed scans are a series of geometry optimizations carried out at 5° intervals as the terminal –OH (of the –$CH_2$OH group (the HOCC dihedral), the –$CH_2$ – (the OCCO dihedral) and the axial/equatorial –OH at C1 (the HOCO dihedral) are rotated. Scans of energy as the rotational angles are changed show that only the orientation of hydroxymethyl substituent at C5 makes any significant contribution to the energy. Rotation about the C-O bond, the HOCO dihedral for the hydroxyl group at C1, shows a low-level variation in energy (~6 kcal range). Similarly, rotation about the C-O bond, the HOCC dihedral in the hydroxymethyl group provides energy changes in the same range. However, rotation about the C5-C6 bond (the OCCO dihedral) show double that range of energies (~12 kcal) and prominent minima indicating the *gg*, *gt*, and *tg* rotamers. Additionally, comparisons of dihedral scans and conformational energies of 2-hydroxymethyl 6-hydroxyl-tetrahydro-*2H*-pyran and 2-hydroxymethyl-tetrahydro-*2H*-pyran with 1,5-anhydro-D-glucitol and glucose indicate that the hydroxyl substituents on the pyran ring make little contribution to the stability of the α–, β– conformers and the *gg*, *gt*, and *tg* rotamers of glucose.

Three-dimensional scans of energy versus the two dihedrals in in the hydroxymethyl group (HOCC and OCCO) were done for both α– and β–D-glucopyranose to develop a potential energy surface to confirm the geometries, energies and number of the low energy structures.